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CFD study of gas mixing efficiency and comparisons with experimental data

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Abstract

The works conducted by FRI are focused on development a new type of mixing devices (burners) for fuel and oxidizer preventing from ignition of the mixture in the mixing domain, designed mainly for partial oxidation process used in chemical technology. The presented results are initial stage data of simulation calculations and experimental results using a laboratory equipment supplied with inert gases under environment conditions. The next stage researches will use real gases (fuel and oxidizer) for studies of pilot plant scale partial oxidation processes.
The aim of the paper is to present some data obtained during process modeling and experiments carried out in the laboratory set for studying efficiency of gas mixing in a mixing chamber and to develop a new geometry of burners for high stream technologies. The experiments have been carried out using inert gases (air and carbon dioxide). Two geometry solutions of mixing chambers have been reported.

Keywords

gas mixing, burner, partial oxidation, CFD calculations

1. Introduction

Mixing of gases is a unit operation widely applied in many industrial branches [1, 2, 3]. The gas mixing process is usually so fast that it does not require any special equipment. It does not regard the case if there are considered fast reacting gases. In that case the mixing process can change the reaction progress and/or produce undesirable side products. One of the case is, considered below, partial oxidation of natural gas. Process of partial oxidation of natural gas (non-catalytic partial oxidation – POX or catalytic autothermal reforming – ATR) is used to produce synthesis gas, basic semi - product for ammonia, methanol, alcohol OXO production as well as synthetic fuels production using Fischer-Tropsch method. Available literature models of ATR reactor focus on the process running only in a catalyst layer. Partial oxidation chamber is modeled using the simplest model - equilibrium model. Validation of the model is based on analysis of near equilibrium product composition.

1.1. Technology of autothermal reforming

ATR process has been used from 9^{th} decade of twenty century as an interesting alternative to steam process reforming – SRM. The ATR process is governed by the following equations [4]:

$$CH_4 + 0.5O_2 = 2H_2 + CO \quad (-\Delta H = 36 \text{ kJ /mol}) \qquad (1)$$

The reactants to the process are: natural gas and oxygen or air enriched with oxygen. Steam and/or carbon dioxide additives allow modifying of product composition and prevents from production of undesirable side product (soot).
In commercial plants using partial oxidation of natural gas it is impossible to avoid full oxidation of part of methane to CO_2 and H_2O:

$$CH_4 + 2O_2 = 2H_2O + CO_2 \quad (-\Delta H = 802 \text{ kJ /mol}) \qquad (2)$$

Steam added to reactants of partial oxidation process reacts with methane and carbon monoxide by the following reactions:

$$CH_4 + H_2O = 3H_2 + CO \quad (-\Delta H = -206 \text{ kJ /mol}) \qquad (3)$$

$$CO + H_2O = H_2 + CO_2 \quad (-\Delta H = 41 \text{ kJ /mol}) \qquad (4)$$

To obtain high efficient transformation of methane the partial oxidation process is carried out at high temperature. In non-catalytic process the required temperature is above 1200 °C, and in catalytic process the temperature is lower and is above 900 °C. For economic reason the partial oxidation processes run at pressure 2 – 4 MPa. The reactor consists of: burner (mixing chamber of reactants), chamber, partial oxidation chamber, catalytic bed.
The burner is a key element of ATR reactor. Its task is to shape the streams of reactants enabling them fast and ideal mixing before entry to partial oxidation chamber. Thus the burner allows to obtain uniform, with respect to temperature and composition, product downstream the partial oxidation chamber.
There are known a few design patterns of burners for partial oxidation: torus shape burner with nozzles for oxygen supply placed in gas stream channel,

burner with circumference slot for natural gas supply and perpendicular slot for oxygen supply, burner with many parallel pipes for oxygen supply placed in gas stream channel, burner with swirling device, burner with gas pre-mixture.
Correctly operating burner produce short symmetrical flame shifted about 5 cm from burner outlet, and not longer than 0.5 m, and not reaching reactor's walls. Flame zone temperature is about 2000 °C. The temperatures are strongly affected by amount of steam supplied to natural gas and oxygen concentration in reactants mixture. The cone shape chamber for partial oxidation of natural gas is of volume providing residence time of 0.5 – 2 s enabling non-catalytic reactions Eq. (1) - (4).

2. Mathematical modeling using CFD tool

CFD tools are developed as university or commercial products such as Fluent or many others [5, 6]. There are a few stages covering the total path of calculations using this tool. The first one is pre-processing which concerns the construction of the geometry (2 or 3 dimensions), generation of a grid, specifying of boundary conditions and fluid properties, and physical and/or chemical phenomena. The second one is solver which calculates the flow variables by solving a system of discretized algebraic equations. The fluent solver uses finite volume method. The third one is post-processing covering also visualisation of data. The solver produces a large amount of data which are stored in the output files. The data can be used for further processing allowing to generate 2D or 3D contour and/or surface plots, vector plots, geometry and mesh plots, and many others.
Generally the solver uses the governing equations of fluid flow comprising the conservation laws of mass, momentum and energy. The set of equations solved by CFD solver is as follows:
the continuity equation:

$$\frac{\partial \rho}{\partial t} + div(\rho \bar{u}) = 0 \tag{6}$$

the momentum equation:

$$\frac{\partial \rho \bar{u}}{\partial t} + div(\rho \bar{u}\bar{u}) = F + div\sigma \tag{7}$$

the energy equation:

$$\frac{\partial}{\partial t}(\rho H) + div(\rho u H) = div(\lambda gradT) + \frac{\partial p}{\partial t} \tag{8}$$

where H is the total enthalpy, ρ is the fluid density, u is the fluid velocity vector, p is the pressure, T is the temperature, t is the time, F is a source, λ is the thermal conductivity, σ is the stress tensor.

The gas flow and mixing phenomena were simulated with a commercial CFD software Fluent 6.2. This finite volume CFD code is widely used for solving transport equations of mass, momentum and energy conservation. In practical cases, in nitrogen industry there are prevailing turbulent flows. To solve the practical problems a turbulence modelling is required. This can be done by adding additional equations for turbulent energy and its dissipation. Chemical reactions running in a chamber of partial oxidation can be studied using calculation approach based on complex reaction mechanisms. The mechanism is based on consideration of 200 to 1000 of elementary reactions with 40 – 100 species and radicals. In the calculations there are considered mixing, diffusion, and stream dynamics. Also, reaction kinetics should be incorporated. To simplify calculations, an instant reaction model may be assumed.

3. Physical modeling of a burner and partial oxidation chamber

Knowledge of reaction mechanism and CFD technique used to model processes in partial oxidation chamber is not a sufficient factor by itself. The model based data should be verified experimentally. An experimental verification of partial oxidation in pilot plant is possible only to some extent – using temperature measurement data, doing post work analysis of a burner, analyzing trace of flame on the chamber wall and catalyst state after experiments. Another measurements within a chamber, in the flame region and under high pressure are impossible from practical point of view. It may be probably assumed that model validation can be carried out only at low temperatures and using substitute media. As a substitute media for “cold” modelling are usually used carbon dioxide and air. Of course, some similarity criteria must be observed to obtain reliable results including residence time of the reactants in the industrial chamber. The main source of errors during modelling of burner and partial oxidation chamber can be effected by rescale, chemical reaction contribution and high pressure (higher gas density). The element of a measurement set designed for burner investigations (mixing chambers) and partial oxidation chamber supplied with cold air and carbon dioxide is shown in Fig. 1. The essential elements of the set are: V-1 chamber and replaceable mixers type M and type R – models of burners for partial oxidation. The chamber is shaped as an inverted cone ended with the short cylindrical part. The mixer is placed at a top part of the cone.

The vertical angle of the cone is 60°, its base diameter is 600 mm. Gas can flow through a free outlet or through the perforated plate of 18 % free surface. A measuring probe was inserted into the chamber to take samples for gas analyzer measuring CO_2 concentration. The stream direction and its value was determined by the flow anemometer. The following burner construction have been tested: "R" - with parallel stream flow, "M" - with mixing stream I and II inside the burner region and directed at angle 45^0 to the output flowing stream.

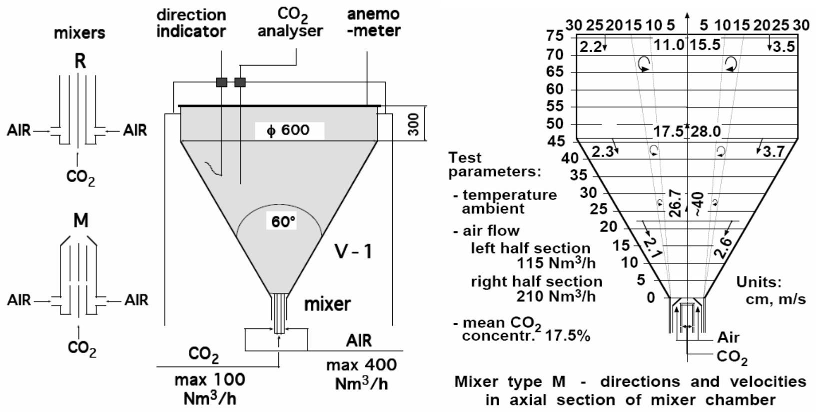

Fig. 1. Experimental setup for measurement of flow and concentration with mixers type M and R.

3.1. Aerodynamic measurements in the partial oxidation chamber

The output stream of circular cross section (from burner) flows into partial oxidation chamber space. The partial oxidation chamber with its vertical angle of 60º is slightly like an open space for the stream flowing out the burner. When flowing stream encounter a bed layer with its hydraulic resistance, the flow pattern changes and some part of gas recirculates. Another part of the gas flows across the porous bed. Recirculation rate is probably high due to high linear gas velocity and its high density in real plant. The experiments have been carried out at two flow rates: 115 and 210 m^3/h and at mean CO_2 concentration of 17.5 vol. %, and at ambient temperature. Gas concentration was measured using sweeping probe across two diameters and at different levels. Flow velocity was measured using an anemometer. In Fig. 1 there are shown radial and longitudinal chamber dimensions in which measurements have been done. Data have been collected using data acquisition system.

4. Results and discussion

Experimental results have been presented in Fig. 2. As an objective function defining efficiency of mixing process a concentration field function defined as follows: $\bar{c}_F = \frac{1}{F}\int_o^F \left(\frac{c}{c_{av}}\right)^2 dF$, where c – actual concentration, c_{av} – average concentration, F – cross sectional area, c_F - concentration field value determining non-uniformity of gas concentration. The values have been calculated for experimental and model data. For R type burner the c_F values are 1.9 – 1.15, and for M type 1.8 – 1.05. There is an information that mixing device of M type is better with respect to the objective functions comparing the R type. The M type mixing device has been recommended for further studies using the flammable gases.

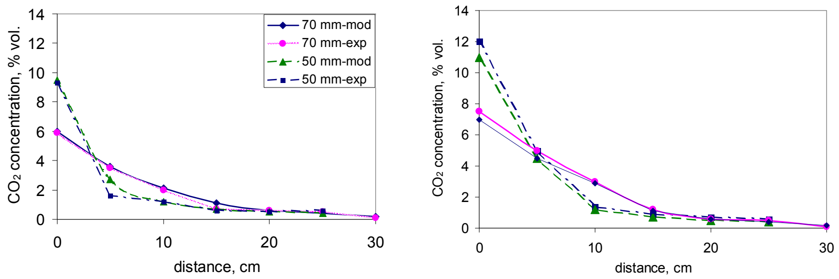

Fig. 2. CO_2 concentration distribution in partial mixing device of M (left) and R (right) type; mod-model, exp - experimental.

5. Conclusions

The obtained results have proved that calculated gas flow patterns are in good conformity with experimental results, Fig.2. The "cold" based measurements can be used as a comparable data particularly for investigating of the burners at initial stage of their development. Also the data can provide a support for validation of CFD calculations. CFD based modeling of mixing processes is a powerful tool for study different types of burners and their properties at different stages of their design.

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